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This grant funded the acquisition of a 128 node/256 processor cluster computer that now supports the computational needs of the combined, Air Force-sponsored research groups of Prof. D. Scott Stewart (PI) in Mechanical Science and Engineering, (MechSE), Prof. John Buckmaster (Co-PI) in Aerospace Engineering (AE), and Thomas L. Jackson (Co-PI) in Computational Science and Engineering (CSE), all at the University of Illinois. The combined Stewart/Buckmaster/Jackson group continues to support advanced explosive system design and advanced propellant combustion and addresses critical areas needed for advanced high energy density devices central to the AF's mission. Stewart is currently supported by grants from AFRL Munitions Directorate and AFOSR/ Physical Mathematics and Applied Analysis (AFOSR/NE).

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For: AFOSR Grant # FA9550-06-1-0332, Final Report
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FINAL REPORT FOR:

"Computational Equipment for Support of Air Force Sponsored Programs for the Design of Advanced and Miniaturized Explosive and Advanced Propellant Systems"

AFOSR Grant # FA9550-06-1-0332
Grant period: May 1 2006 to May 1 2007

Submitted by

D. Scott Stewart, University of Illinois, Mechanical Science and Engineering, PI
John D. Buckmaster, University of Illinois, Aerospace Engineering, Co-PI
Thomas L. Jackson, University of Illinois, Computation Sci. & Engineering, Co-PI

PROJECT SUMMARY

This grant funded the acquisition of a 128 node/256 processor cluster computer that now supports the computational needs of the combined, Air Force-sponsored research groups of Prof. D. Scott Stewart (PI) in Mechanical Science and Engineering, (MechSE), Prof. John Buckmaster (Co-PI) in Aerospace Engineering (AE), and Thomas L. Jackson (Co-PI) in Computational Science and Engineering (CSE), all at the University of Illinois. The combined Stewart/Buckmaster/Jackson group continues to support advanced explosive system design and advanced propellant combustion and addresses critical areas needed for advanced high energy density devices central to the AF's mission. Stewart is currently supported by grants from AFRL Munitions Directorate and AFOSR/ Physical Mathematics and Applied Analysis (AFOSR/NE). Buckmaster and Jackson are supported independently by AFOSR/NE.

Stewart's group in Mechanical Science and Engineering (MechSE) uses the equipment to carryout research simulations to model critical scientific experiments related to explosives devices of interest to the Munitions Directorate, (AFRL/RW), Eglin AFB, such as adaptable munitions, miniature and micro-munitions efforts and other new systems, in collaboration with AFRL/RW and other designated research teams. The simulations of shock and detonation physics are fully three dimensional (3D), multi-scale, multi-phase, involve high-pressure, high-density multi-material interactions, and require facilities to carry out large-scale calculations. The Buckmaster/Jackson group are engaged in carrying out large-scale, 3D, multi-material simulations of low Mach number burning of heterogeneous propellants of current interest to AFRL's Propulsion Directorate, Space and Missile Propulsion Division and AF supported contractors. These simulations require long term averaging of the burning of propellant beds and need computations on a fast, parallel computational platform with rapid turnaround for optimization. Full reporting on the research accomplishments associated with the supporting AF

grants is available by requests directed to (D. S. Stewart) dss@uiuc.edu, J. D. Buckmaster (limey@uiuc.edu) or T. L. Jackson (tlj@cse.uiuc.edu), and are recorded in other filed technical reports.

The equipment is currently being used to help graduate students, postdocs, collaborating AF scientists and other AF-sponsored collaborators carry out and learn parallel, multi-scale simulation techniques, and perform high-level research in multi-scale theory and simulation that supports AF efforts in the areas of complex reactive flows described above.

Summary Overview of the Purchase and Installation of the Equipment

The request and acquisition of equipment was for 128 Apple G5 dual processor nodes (for a total of 256 processors) with 4 Gbytes RAM/node (for a total RAM of 1 Terabyte), a Myrianet Switch that connected the processors, a RAID disk farm, rack mounts, peripherals and Apple Care Support for three years. In addition the initial request included the purchase of one Apple Intel laptop computer system and monitor for each of the Pis, for code preparation and system oversight.

The AF DURIP grant provided approximately $512,899, that was combined with an additional cost share contribution of $188,164, comprised of an Apple Corporation donation of $76,080 and a State of Illinois matching fund contribution of $112,084. The total value of the purchased equipment and installation was over $700,000. Detailed accounting is available from Mr. John Weirschem (Business Manager), MechSE jwiersch@uiuc.edu, and copies of purchase vouchers can be made available on request. These funds were expended on the equipment described in the previous paragraph, plus some additional peripheral equipment. A request has been made to expend small amount of remaining State match funds to purchase a small workstation cluster for preparing code for the large-scale cluster (as of 5/01/08).

The grant starting date was officially 5/1/2006. A detailed plan for purchase acquisition of Apple equipment, compatible with an existing Apple cluster installation, “Turing” established by the College of Engineering (COE) and maintained by staff in the CSE program. Specifically D. S. Stewart and T. L. Jackson worked with Mr. William Dick (Associate Director of CSE) and his staff to make the final purchase order, and carry out the installation. The equipment orders were placed starting in July 2006, through October 2006. The AF DURIP G5 nodes were installed in the COE machine room in the “Digital Equipment Laboratory Building” on the north side of Springfield Avenue, of the main campus of the University of Illinois, in Urbana, IL. See Figure 1. The 256 processors, Myrianet switch and RAID which defines the supercomputer cluster, became fully operational in early calendar year 2007 and at that time the first “research” production runs on the DURIP cluster were carried out by the Jackson group.

Note that the 256 AF/DURIP processors are linked to another set of 256 processors to provide a total block of 512 contiguous processors that can be made available to any user of the system. In addition the Turing cluster has yet another 1024 processors available to users through a separate switch.

The Stewart/Buckmaster/Jackson user group has highest priority on the systems and their jobs always run first. If nodes are not being used they become available to a larger “Turing” user

community. In exchange for general user access to the AF-purchased nodes, the AF/DURIP cluster segment receives software support as part of the COE contributed maintenance. Our use (Stewart/Buckmater/Jackson) has been essentially software/hardware maintenance free since the nodes were installed. We believe our acquisition choices to work with the COE and CSE were the correct ones and we have been satisfied with the arrangements.

A photograph of the AF cluster (of Stewart, co-workers and students, taken 8/10/2007) is shown in Figure 1.

Figure 1. AF DURIP G5 nodes and cabling, being inspected and discussed by D. S. Stewart and members of the Stewart research group. Left to right (Brian Taylor, D. Scott Stewart, Juan Saenz and Dr. Sunhee Yoo.) Picture taken August 10, 2007, copyright Board of Trustees, University of Illinois.

Laboratory for Simulation and Modeling of Energetic Materials

Given the acquisition of the AF/DURIP sponsored cluster as the top end machine, D. Scott Stewart established a new computational laboratory, named ***"Laboratory for Simulation and Modeling of Energetic Materials"*** in the Department of Mechanical Science and Engineering. Figure 2. shows the header page of the new website (under development) that announces our capabilities.

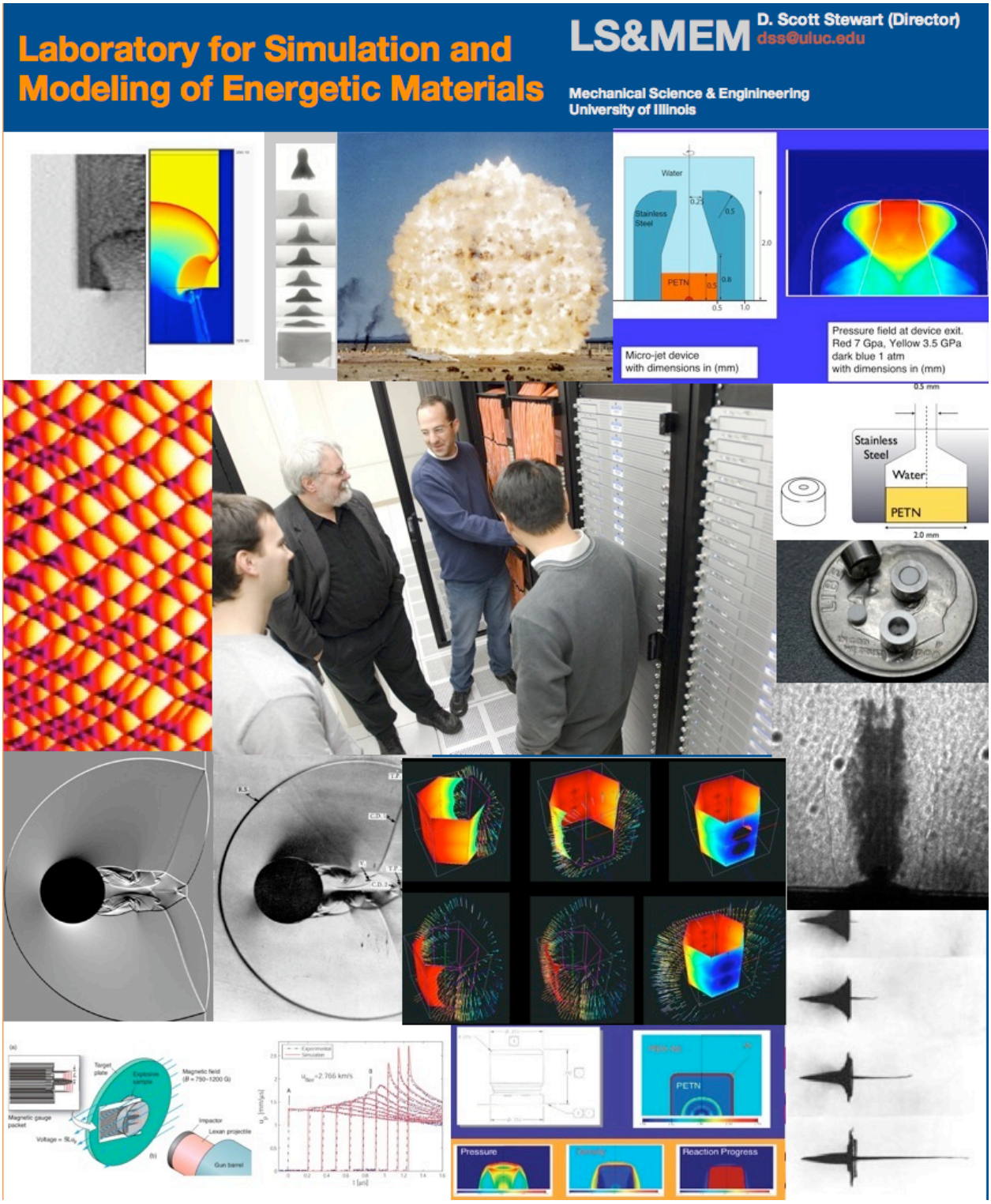

Figure 2. Web page announcement of the "Laboratory for Simulation and Modeling of Energetic Materials" (LS&MEM) in MechSE at U of Illinois. Representative AF/ energetic material applications studied in the Stewart-group are shown. The center inset prominently displays the new G5 cluster computer.

Final Remarks and Further Information

Issues related to Illinois State matching funds delayed the prompt filing of this report. Apologies are tendered to AFOSR and Dr. Nachman. Their generous support and patience and high quality program management is gratefully acknowledged. We also want to acknowledge the generous financial, technical support and encouragement of the Air Force Research Laboratory's Muntions (AFRL/RW) and Propulsion (AFRL/PR) Directorates.

Further information and or detailed accounting is available from Mr. John Wierschem in the MechSE business office at 217 333 6741, jwiersch@uiuc.edu or D. Scott Stewart, dss@uiuc.edu.